4,4'-Methylenedianiline

101-77-9 | DTXSID6022422

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 368 °C

Global applicability domain: Inside

Local applicability domain index: 5.56e-01

Confidence level: 5.76e-01

Nearest Neighbors from the Training Set

Image not found
4,4'-Methylenedianiline
Measured: 398
Predicted: 368

Image not found
Benzidine
Measured: 401
Predicted: 367

Image not found
2,4'-Biphenyldiamine
Measured: 363
Predicted: 367

Image not found
1,2-Benzenediamine,N-phenyl-
Measured: 313
Predicted: 363

Image not found
N-Phenyl-1,4-benzenediamine
Measured: 354
Predicted: 363